



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:19 PM UTC

PDB ID : 6ZFP / pdb_00006zfp
EMDB ID : EMD-11185
Title : Cryo-EM structure of DNA-PKcs (State 2)
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-17
Resolution : 3.24 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

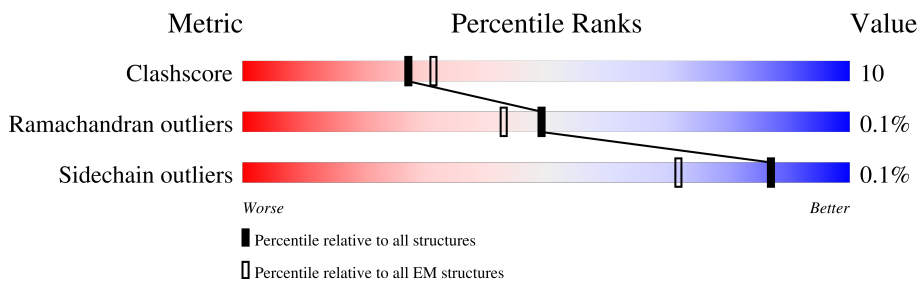
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	4156	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29385 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

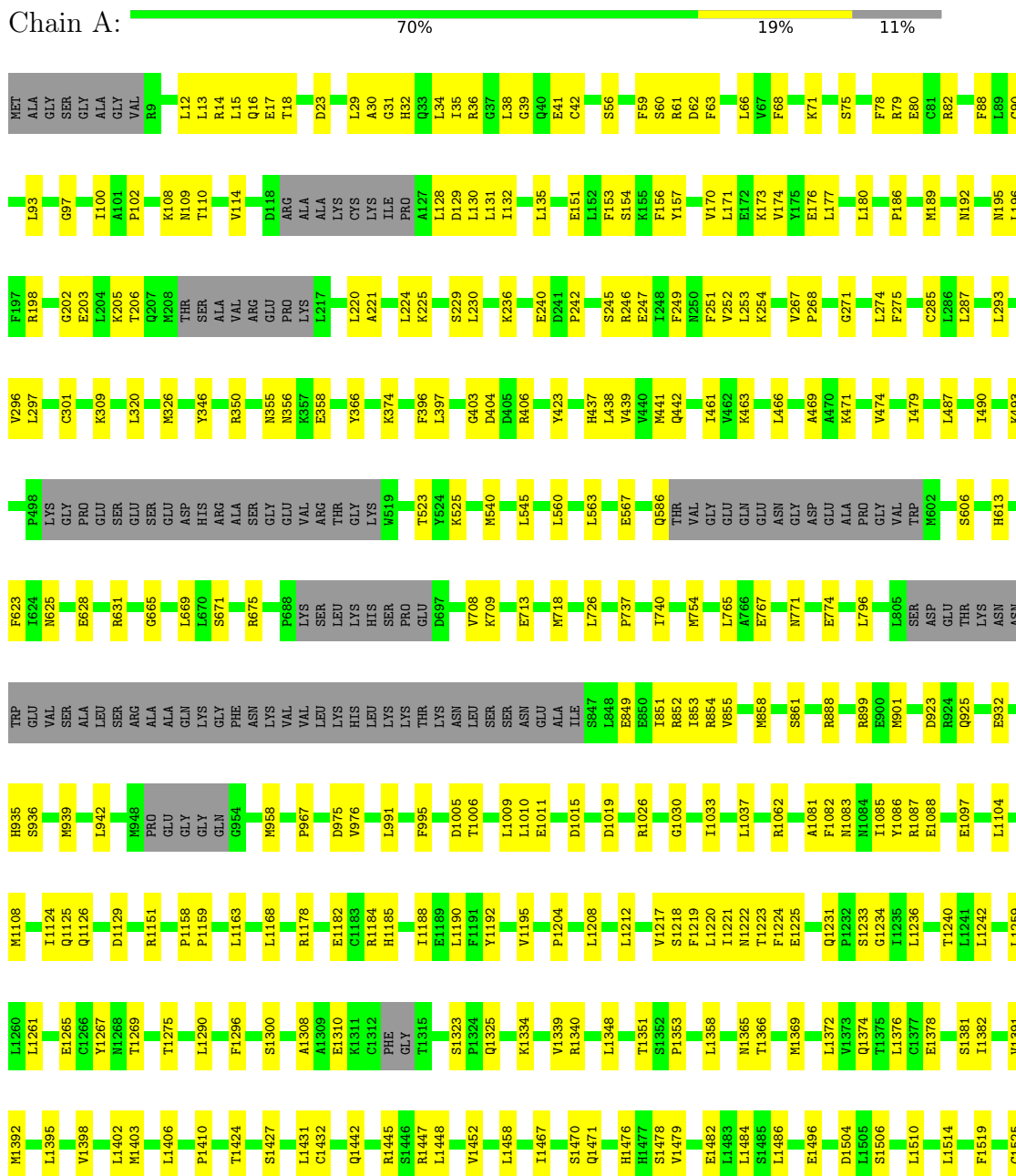
- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-PKcs, DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3704	29385	18849	4964	5379	193	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-PKCs,DNA-PKCs



R3167	K3009	K2824	S2489	D2376	I2256	SER	K1985	F1814	T1643	E1526
M3176	E3012	E2828	D2492	L2385	K2259	VAL	ARG	T1815	K1642	R1527
I3182	E3013	I2832	D2493	F2260	F2260	F2119	ARG	Q1816	I1652	L1528
R3186	E3014	E2832	D2494	F2389	G2262	L2121	ASN	R1817	D1685	L1532
C3187	S3015	S2849	I2498	V2392	D2269	L2133	PRO	F1819	K1689	L1538
K3196	E3033	F2854	L2517	L2396	N2270	L2145	VAL	V1820	G1690	A1541
L3197	F3034	C2857	R2522	C2397	S2271	F2145	GLY	D1821	G1690	SER
THR	S3047	C2863	ALA	V2400	V2272	K2148	GLY	L1824	V1693	LEU
PRO	L3053	C2863	L2531	L2277	L2277	I2151	GLN	L1827	L1710	GLY
LEU	L3062	S2877	T2535	R2404	V2280	I2151	ASP	L1828	R1711	SER
PRO	L3062	L2884	E2406	V2405	M2281	E2155	PRO	L1836	R1711	GLN
GLU	D3066	L2884	G2407	E2406	M2281	E2155	ARG	L1837	L1714	GLY
ASP	K3067	P2887	M2408	G2407	C2292	R2158	LYS	E1837	E1715	S1549
ASN	I3077	E2895	L2542	L2411	Q2301	W2164	LYS	E1838	I1718	V1550
SER	L3078	E2895	E2551	F2412	Q2301	L2165	THR	D1864	F1553	
VAL	L3088	P2902	A2558	F2413	L2165	S2166	ILE	F1722	F1722	
ASP	L3091	ALA	T2559	Q2414	S2166	P2167	ARG	S1726	S1726	
GLY	L3092	LEU	N2560	L2415	L2168	L2169	ARG	M1871	G1732	Y1560
ASP	L3093	GLY	L2562	F2420	S2308	L2169	GLY	Y1874	T1733	S1561
PRO	L3094	GLY	L2562	F2420	S2308	L2169	GLY	K1875	R1735	L1562
ASP	L3095	GLY	L2562	F2420	S2308	L2169	GLY	M1880	G1735	I1567
ASP	L3096	GLY	L2562	F2420	S2308	L2169	GLY	Q1754	Q1754	E1570
ARG	L3097	GLY	L2562	F2420	S2308	L2169	GLY	R1883	M1757	L1571
GLY	L3098	GLY	L2562	F2420	S2308	L2169	GLY	N1897	L1758	L1572
GLY	L3099	GLY	L2562	F2420	S2308	L2169	GLY	L1758	L1758	K1573
GLY	L3100	GLY	L2562	F2420	S2308	L2169	GLY	E1760	E1760	L1575
GLY	L3101	GLY	L2562	F2420	S2308	L2169	GLY	T1912	E1769	S1585
GLY	L3102	GLY	L2562	F2420	S2308	L2169	GLY	I1916	Q1770	S1586
GLY	L3103	GLY	L2562	F2420	S2308	L2169	GLY	Y1920	F1782	N1589
GLY	L3104	GLY	L2562	F2420	S2308	L2169	GLY	L1933	I1785	T1590
GLY	L3105	GLY	L2562	F2420	S2308	L2169	GLY	L1934	A1786	M1592
GLY	L3106	GLY	L2562	F2420	S2308	L2169	GLY	E1935	R1788	Q1614
GLY	L3107	GLY	L2562	F2420	S2308	L2169	GLY	R1936	G1789	K1617
GLY	L3108	GLY	L2562	F2420	S2308	L2169	GLY	R1937	S1790	L1618
GLY	L3109	GLY	L2562	F2420	S2308	L2169	GLY	R1938	T1793	I1622
GLY	L3110	GLY	L2562	F2420	S2308	L2169	GLY	L1939	Q1794	I1622
GLY	L3111	GLY	L2562	F2420	S2308	L2169	GLY	Y1940	Q1794	V1795
GLY	L3112	GLY	L2562	F2420	S2308	L2169	GLY	F1961	G1796	K1627
GLY	L3113	GLY	L2562	F2420	S2308	L2169	GLY	Y1962	L1797	K1627
GLY	L3114	GLY	L2562	F2420	S2308	L2169	GLY	Q1963	V1602	V1632
GLY	L3115	GLY	L2562	F2420	S2308	L2169	GLY	S1968	R1806	V1633
GLY	L3116	GLY	L2562	F2420	S2308	L2169	GLY	L1975	R1806	K1635
GLY	L3117	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	D1636
GLY	L3118	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3119	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3120	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3121	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3122	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3123	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3124	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3125	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3126	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3127	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3128	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3130	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3131	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3132	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3133	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3134	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3135	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3136	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3137	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3138	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3139	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3146	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3147	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3148	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3149	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3150	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3151	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3152	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3153	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3154	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3155	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3156	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3157	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3163	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3164	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3165	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3166	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3175	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3178	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3180	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3195	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
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GLY	L3197	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3198	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3199	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3200	GLY	L2562	F2420	S2308	L2169	GLY	L1976	L1812	E1640
GLY	L3201	GLY								

L4051	V3868	K3665	N3551	D3271
I4059	E3875	L3666	V3555	C3281
L4064	V3878	M3670	K3561	S3284
Y4077	P3879	L3680	L3575	SER
A4081	A3880	K3681	E3582	VAL
R4090	D3881	E3682	L3583	ILE
Q4103	L3882	S3684	V3568	ASP
L4107	L3883	P3685	K3568	SER
M4108	A3886	K3687	L3596	ALA
D4113	R3889	V3692	L3596	GLU
W4127	E3895	E3700	V3601	L3439
M4128	I3913	K3710	N3602	A3444
X5009	T3917	P3711	K3603	L3445
X6020	T3917	E3714	N3604	V3446
	D3922	E3714	N3605	V3447
	R3923	R3718	E3607	E3448
	H3924	F3722	K3608	K3449
	L3925	D3723	E3611	M3450
	N3926	E3724	N3612	L3456
	I3938	L3751	K3613	Y3315
	H3944	S3779	A3616	L3316
	M3959	A3780	G3617	S3317
	P3960	R3789	G3618	K3318
	F3961	R3789	A3622	A3322
	K3975	T3790	L3625	E3477
	Y3981	Y3791	G3626	L3329
	A3987	S3792	A3627	T3333
	R3992	V3793	F3628	L3482
	M4000	M3796	R3629	M3483
	M4015	L3602	I3633	T3484
	M4015	L3803	F3636	L3348
	Q4018	L3806	E3639	E3352
	K4019	L3816	H3643	D3369
	M4020	T3819	K3646	Q3383
	K4023	L3829	K3650	E3387
	Q4024	L3843	K3655	A3396
	W4027	M3846	L3656	GLN
	E4030	M3858	S3657	PRD
	K4050	R3864	D3661	SER
			N3664	TRP
				SER
				PRD
				TRP
				SER
				CYS
				GLY
				P3406
				I3410
				K3414
				R3425
				M3430
				ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/29848	0.40	1/40366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3483	MET	N-CA-C	8.44	121.23	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29385	0	29509	545	0
All	All	29385	0	29509	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ($\text{\AA}$)	Clash overlap ($\text{\AA}$)
1:A:3444:ALA:HA	1:A:3482:LEU:CD2	1.99	0.93
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3444:ALA:O	1:A:3482:LEU:HD21	1.83	0.79
1:A:899:ARG:HE	1:A:2568:MET:HB2	1.48	0.78
1:A:403:GLY:H	1:A:406:ARG:HH12	1.29	0.78
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.69	0.75
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.71	0.73
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.21	0.73
1:A:3298:LEU:HD12	1:A:3333:THR:HG23	1.69	0.73
1:A:3444:ALA:CA	1:A:3482:LEU:CD2	2.66	0.72
1:A:1933:LEU:HD13	1:A:1936:ARG:HB3	1.71	0.72
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.20	0.71
1:A:3444:ALA:HB1	1:A:3482:LEU:HD22	1.72	0.71
1:A:356:ASN:ND2	1:A:404:ASP:O	2.24	0.71
1:A:3444:ALA:CB	1:A:3482:LEU:HD22	2.21	0.71
1:A:2151:ILE:HG21	1:A:2188:GLU:HG2	1.73	0.71
1:A:3520:GLU:OE2	1:A:3524:ASN:ND2	2.25	0.70
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.62	0.70
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.56	0.69
1:A:767:GLU:HG2	1:A:851:ILE:HD11	1.75	0.69
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.25	0.69
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.65	0.69
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.26	0.68
1:A:3186:ARG:HD3	1:A:3238:MET:HE1	1.75	0.68
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.75	0.68
1:A:936:SER:OG	1:A:2773:ARG:NH1	2.27	0.68
1:A:1484:LEU:HD11	1:A:1527:ARG:HH12	1.57	0.68
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.74	0.68
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.75	0.68
1:A:709:LYS:NZ	1:A:713:GLU:OE2	2.27	0.67
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.27	0.66
1:A:75:SER:H	1:A:78:PHE:HB3	1.59	0.66
1:A:1369:MET:HE1	1:A:1406:LEU:HD11	1.77	0.66
1:A:3495:PHE:HB3	1:A:3502:MET:HE1	1.75	0.66
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.26	0.66
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.29	0.66
1:A:38:LEU:O	1:A:41:GLU:HB3	1.95	0.66
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.78	0.66
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.76	0.65
1:A:1432:CYS:HB3	1:A:1486:LEU:HD11	1.79	0.65
1:A:774:GLU:HG2	1:A:858:MET:HE3	1.79	0.64
1:A:90:CYS:O	1:A:93:LEU:HB3	1.98	0.64
1:A:93:LEU:O	1:A:97:GLY:N	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2365:ASN:HD22	1:A:2396:LEU:HD13	1.63	0.64
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.31	0.64
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.79	0.63
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.81	0.63
1:A:3924:HIS:ND1	1:A:3926:ASN:OD1	2.29	0.63
1:A:3009:LYS:O	1:A:3013:TYR:HB3	1.98	0.63
1:A:173:LYS:HA	1:A:176:GLU:HG3	1.81	0.63
1:A:374:LYS:HD2	1:A:423:TYR:HB3	1.82	0.62
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.82	0.62
1:A:3444:ALA:HA	1:A:3482:LEU:HD21	1.82	0.62
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.80	0.61
1:A:2169:LEU:HD11	1:A:2215:LEU:HD22	1.80	0.61
1:A:2439:ILE:O	1:A:2443:MET:HG3	2.00	0.61
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.34	0.61
1:A:3448:GLU:HB3	1:A:3482:LEU:HD11	1.81	0.61
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.33	0.61
1:A:186:PRO:HA	1:A:189:MET:HE1	1.83	0.61
1:A:2155:GLU:OE2	1:A:2158:ARG:NH2	2.34	0.60
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.35	0.60
1:A:2195:SER:O	1:A:5009:UNK:N	2.34	0.60
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.17	0.60
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.67	0.60
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.01	0.60
1:A:3477:GLU:HA	1:A:3477:GLU:OE1	2.01	0.60
1:A:3425:ARG:NH1	1:A:4000:ASN:OD1	2.35	0.60
1:A:2406:GLU:OE1	1:A:2441:LYS:NZ	2.34	0.59
1:A:4023:LYS:HG2	1:A:4024:GLY:H	1.67	0.59
1:A:1358:LEU:HD11	1:A:1410:PRO:HG2	1.84	0.59
1:A:3639:GLU:O	1:A:3643:HIS:N	2.28	0.59
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.35	0.59
1:A:3444:ALA:CA	1:A:3482:LEU:HD21	2.33	0.59
1:A:3646:LYS:H	1:A:3650:LYS:HB3	1.68	0.59
1:A:131:LEU:HD22	1:A:173:LYS:HD2	1.85	0.59
1:A:1871:MET:HG2	1:A:1940:TYR:HA	1.85	0.58
1:A:3444:ALA:HB2	1:A:3478:GLU:HG2	1.85	0.58
1:A:3154:GLN:OE1	1:A:3226:ASP:N	2.37	0.58
1:A:1125:GLN:NE2	1:A:1129:ASP:OD2	2.37	0.58
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.85	0.58
1:A:2091:HIS:CE1	1:A:2093:CYS:SG	2.96	0.58
1:A:2357:GLU:HB3	1:A:2385:LEU:HD21	1.85	0.58
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.29	0.58
1:A:203:GLU:O	1:A:206:THR:OG1	2.20	0.58
1:A:1975:LEU:HD12	1:A:1976:LEU:HD12	1.86	0.58
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.36	0.58
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.37	0.57
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.39	0.57
1:A:205:LYS:HG2	1:A:249:PHE:HZ	1.70	0.57
1:A:628:GLU:OE2	1:A:631:ARG:NH2	2.37	0.57
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	1.86	0.57
1:A:2361:ILE:HD12	1:A:2389:PHE:HE2	1.67	0.57
1:A:1376:LEU:HD22	1:A:1403:MET:HE1	1.86	0.57
1:A:606:SER:OG	1:A:1026:ARG:NH2	2.37	0.56
1:A:108:LYS:HZ2	1:A:156:PHE:HZ	1.52	0.56
1:A:229:SER:HA	1:A:274:LEU:HD13	1.88	0.56
1:A:718:MET:HE3	1:A:726:LEU:HD11	1.86	0.56
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.38	0.56
1:A:3796:MET:HE2	1:A:3802:LEU:HG	1.87	0.56
1:A:3961:PHE:HE2	1:A:4107:LEU:HD13	1.70	0.56
1:A:2260:PHE:O	1:A:2270:ASN:ND2	2.38	0.56
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.37	0.56
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.37	0.56
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.70	0.56
1:A:1011:GLU:O	1:A:1015:ASP:N	2.38	0.56
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.24	0.56
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.88	0.56
1:A:205:LYS:HG2	1:A:249:PHE:CZ	2.41	0.56
1:A:901:MET:SD	1:A:2535:THR:OG1	2.64	0.56
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.78	0.56
1:A:3751:LEU:HD22	1:A:3803:ILE:HD11	1.87	0.56
1:A:1754:GLN:HG3	1:A:1785:ILE:HG13	1.88	0.56
1:A:1541:ALA:HB2	1:A:1550:VAL:HG12	1.87	0.56
1:A:1819:PHE:O	1:A:1823:SER:OG	2.22	0.56
1:A:1961:PHE:O	1:A:1961:PHE:CD1	2.59	0.56
1:A:2224:PHE:HB2	1:A:2272:VAL:HG11	1.87	0.56
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.33	0.56
1:A:1867:ILE:O	1:A:1871:MET:HG3	2.06	0.55
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.54	0.55
1:A:771:ASN:OD1	1:A:854:ARG:NH2	2.40	0.55
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.55	0.55
1:A:1828:LEU:HD22	1:A:1880:MET:HE3	1.89	0.55
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:GLN:HG3	1:A:1445:ARG:HH12	1.71	0.55
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.39	0.55
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.46	0.55
1:A:56:SER:HA	1:A:59:PHE:CD2	2.42	0.55
1:A:1484:LEU:HD11	1:A:1527:ARG:NH1	2.22	0.55
1:A:1759:LEU:HD12	1:A:1785:ILE:HD13	1.88	0.55
1:A:2168:LEU:HD22	1:A:2189:ILE:HD11	1.89	0.55
1:A:3608:LYS:O	1:A:3611:GLU:HG3	2.07	0.55
1:A:849:GLU:OE1	1:A:3108:GLN:NE2	2.38	0.54
1:A:3605:ASN:OD1	1:A:3606:ILE:N	2.40	0.54
1:A:4027:TRP:HE3	1:A:4030:GLU:HB3	1.72	0.54
1:A:129:ASP:OD1	1:A:129:ASP:N	2.40	0.54
1:A:1267:TYR:HD2	1:A:1290:LEU:HD22	1.72	0.54
1:A:2411:LEU:HD11	1:A:2415:LEU:HD23	1.90	0.54
1:A:932:GLU:OE2	1:A:2771:LEU:HD13	2.08	0.54
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.72	0.54
1:A:131:LEU:O	1:A:135:LEU:HG	2.08	0.54
1:A:1920:TYR:HE1	1:A:1963:GLN:CB	2.20	0.54
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.90	0.54
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.88	0.54
1:A:1920:TYR:CE1	1:A:1963:GLN:CB	2.91	0.54
1:A:2148:LYS:HD3	1:A:2185:MET:HE1	1.90	0.54
1:A:267:VAL:HG23	1:A:268:PRO:HD3	1.90	0.54
1:A:79:ARG:HA	1:A:82:ARG:HB2	1.90	0.53
1:A:3575:LEU:HD12	1:A:3796:MET:HE1	1.88	0.53
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.91	0.53
1:A:2474:TYR:HD2	1:A:2517:LEU:HD12	1.74	0.53
1:A:2281:MET:HE1	1:A:2326:ILE:HA	1.90	0.53
1:A:3627:ALA:HB3	1:A:3683:CYS:HB2	1.90	0.53
1:A:1815:THR:O	1:A:1818:SER:OG	2.25	0.53
1:A:56:SER:HA	1:A:59:PHE:HD2	1.73	0.53
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.90	0.53
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	1.90	0.53
1:A:1812:LEU:O	1:A:1815:THR:N	2.36	0.53
1:A:2918:PRO:HB2	1:A:2922:ARG:HH22	1.73	0.53
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.91	0.53
1:A:2091:HIS:HE1	1:A:2093:CYS:SG	2.32	0.53
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.38	0.53
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.09	0.53
1:A:1108:MET:HE1	1:A:1190:LEU:HD22	1.91	0.53
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:SER:O	1:A:1585:SER:OG	2.27	0.52
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.24	0.52
1:A:2933:ILE:HD11	1:A:3121:LEU:HD22	1.91	0.52
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.91	0.52
1:A:3348:LEU:O	1:A:3352:GLU:HG2	2.09	0.52
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.91	0.52
1:A:3097:ASP:OD1	1:A:3098:ARG:N	2.37	0.52
1:A:3444:ALA:C	1:A:3482:LEU:HD21	2.33	0.52
1:A:1519:PHE:CG	1:A:1570:GLU:HG3	2.45	0.52
1:A:3496:ILE:HD11	1:A:3521:ILE:HD11	1.92	0.52
1:A:170:VAL:O	1:A:171:LEU:HD22	2.10	0.52
1:A:2205:VAL:HB	1:A:2208:ASP:HB2	1.92	0.52
1:A:1710:LEU:HG	1:A:1757:MET:HE1	1.92	0.52
1:A:2121:ASP:OD1	1:A:2121:ASP:N	2.43	0.52
1:A:2457:PRO:O	1:A:2460:GLU:HG2	2.10	0.52
1:A:3053:LEU:HD11	1:A:3088:LEU:HD13	1.92	0.52
1:A:3414:MET:HE3	1:A:3414:MET:HA	1.92	0.52
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.45	0.52
1:A:23:ASP:HA	1:A:30:ALA:HB1	1.93	0.51
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.92	0.51
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.11	0.51
1:A:13:LEU:O	1:A:14:ARG:NE	2.43	0.51
1:A:1378:GLU:HG2	1:A:1378:GLU:O	2.10	0.51
1:A:1586:SER:O	1:A:1632:TRP:NE1	2.43	0.51
1:A:708:VAL:HG22	1:A:740:ILE:HG23	1.92	0.51
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.28	0.51
1:A:251:PHE:HA	1:A:254:LYS:HZ2	1.75	0.51
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.76	0.51
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.93	0.51
1:A:1726:SER:O	1:A:1726:SER:OG	2.27	0.51
1:A:2256:ILE:HG22	1:A:2260:PHE:HE2	1.76	0.51
1:A:2424:MET:HE1	1:A:2439:ILE:HD11	1.92	0.51
1:A:3137:GLU:CD	1:A:3186:ARG:HE	2.19	0.51
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.11	0.51
1:A:1037:LEU:HD23	1:A:1085:ILE:HB	1.93	0.50
1:A:1934:LEU:O	1:A:1938:ARG:N	2.43	0.50
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.25	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB3	1.94	0.50
1:A:2259:LYS:HB3	1:A:2272:VAL:HG23	1.94	0.50
1:A:242:PRO:O	1:A:245:SER:OG	2.24	0.50
1:A:1532:LEU:HD11	1:A:1560:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1871:MET:HE1	1:A:1936:ARG:HH21	1.76	0.50
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.12	0.50
1:A:1192:TYR:HH	1:A:1275:THR:HG1	1.58	0.50
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.93	0.50
1:A:2368:THR:HG23	1:A:2372:PRO:HA	1.93	0.50
1:A:2522:ARG:HG2	1:A:2561:PHE:HE1	1.76	0.50
1:A:3944:HIS:NE2	1:A:4020:MET:SD	2.85	0.50
1:A:59:PHE:HB3	1:A:63:PHE:CE1	2.47	0.50
1:A:242:PRO:C	1:A:246:ARG:HE	2.20	0.50
1:A:1374:GLN:HE22	1:A:1381:SER:HB3	1.76	0.50
1:A:3444:ALA:CA	1:A:3482:LEU:HD22	2.42	0.49
1:A:1817:GLN:OE1	1:A:1936:ARG:NH2	2.41	0.49
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.93	0.49
1:A:403:GLY:O	1:A:406:ARG:NH1	2.46	0.49
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.94	0.49
1:A:1470:SER:HB3	1:A:1476:HIS:CD2	2.48	0.49
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.94	0.49
1:A:1006:THR:HG22	1:A:1009:LEU:HB2	1.94	0.49
1:A:1208:LEU:HD21	1:A:1220:LEU:HD11	1.94	0.49
1:A:2584:CYS:SG	1:A:2585:GLU:N	2.85	0.49
1:A:3062:LEU:HD13	1:A:3093:GLN:NE2	2.28	0.49
1:A:301:CYS:O	1:A:309:LYS:NZ	2.38	0.49
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.95	0.49
1:A:36:ARG:HH21	1:A:39:GLY:HA3	1.76	0.49
1:A:1557:GLU:HA	1:A:1592:MET:HE1	1.94	0.49
1:A:2463:SER:O	1:A:2463:SER:OG	2.31	0.49
1:A:3446:VAL:O	1:A:3450:MET:HG2	2.13	0.49
1:A:2261:SER:OG	1:A:2262:GLY:N	2.46	0.48
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.13	0.48
1:A:397:LEU:HD21	1:A:438:LEU:HD22	1.95	0.48
1:A:2415:LEU:HD12	1:A:2420:PHE:CD1	2.48	0.48
1:A:923:ASP:C	1:A:925:GLN:H	2.21	0.48
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.42	0.48
1:A:3227:ILE:HD12	1:A:3227:ILE:H	1.78	0.48
1:A:3444:ALA:HA	1:A:3482:LEU:HD23	1.92	0.48
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.94	0.48
1:A:3104:GLN:OE1	1:A:3139:GLN:NE2	2.46	0.48
1:A:3151:LEU:HD21	1:A:3197:LEU:HA	1.95	0.48
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.47	0.48
1:A:975:ASP:OD1	1:A:976:VAL:N	2.45	0.48
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2301:GLN:OE1	1:A:2305:ASN:ND2	2.46	0.48
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.48	0.48
1:A:2786:LYS:O	1:A:2788:SER:N	2.47	0.48
1:A:3313:SER:HA	1:A:3316:LEU:HB2	1.96	0.48
1:A:253:LEU:HD11	1:A:271:GLY:HA3	1.94	0.48
1:A:1339:VAL:HG23	1:A:1398:VAL:HG21	1.95	0.48
1:A:12:LEU:O	1:A:16:GLN:HG2	2.14	0.47
1:A:1912:THR:O	1:A:1916:ILE:HG12	2.14	0.47
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.48	0.47
1:A:2097:LEU:HD12	1:A:2145:PHE:HZ	1.78	0.47
1:A:2304:VAL:HG12	1:A:2323:LEU:HD11	1.96	0.47
1:A:346:TYR:HB3	1:A:350:ARG:HH12	1.78	0.47
1:A:1323:SER:O	1:A:1325:GLN:N	2.48	0.47
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.96	0.47
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.45	0.47
1:A:63:PHE:O	1:A:66:LEU:HB2	2.15	0.47
1:A:439:VAL:O	1:A:442:GLN:HB3	2.15	0.47
1:A:1009:LEU:HD21	1:A:1062:ARG:NH1	2.29	0.47
1:A:1933:LEU:HD12	1:A:1937:ARG:HG3	1.96	0.47
1:A:1231:GLN:O	1:A:1233:SER:N	2.47	0.47
1:A:1793:THR:O	1:A:1797:LEU:HG	2.15	0.47
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.14	0.47
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.48	0.47
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.47
1:A:942:LEU:HD11	1:A:991:LEU:HD21	1.97	0.47
1:A:14:ARG:O	1:A:18:THR:HG23	2.15	0.47
1:A:540:MET:SD	1:A:540:MET:N	2.88	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.15	0.46
1:A:2107:SER:O	1:A:2107:SER:OG	2.32	0.46
1:A:1711:ARG:NH2	1:A:1760:GLU:OE1	2.48	0.46
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.41	0.46
1:A:1484:LEU:HD21	1:A:1527:ARG:HH22	1.80	0.46
1:A:2940:ARG:HG2	1:A:2957:LEU:HD22	1.95	0.46
1:A:1836:LEU:HA	1:A:1880:MET:HE1	1.97	0.46
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.48	0.46
1:A:195:ASN:O	1:A:198:ARG:HG3	2.15	0.46
1:A:1572:LEU:HD21	1:A:1618:LEU:HD22	1.96	0.46
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	2.15	0.46
1:A:3444:ALA:HB2	1:A:3478:GLU:CG	2.44	0.46
1:A:3449:LYS:HD3	1:A:3449:LYS:HA	1.72	0.46
1:A:726:LEU:HD21	1:A:754:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:SER:O	1:A:3167:ARG:NH1	2.46	0.46
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.16	0.46
1:A:3100:LYS:HB3	1:A:3100:LYS:HE3	1.77	0.46
1:A:100:ILE:HB	1:A:102:PRO:HD3	1.98	0.46
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.31	0.46
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.16	0.46
1:A:2361:ILE:HD12	1:A:2389:PHE:CE2	2.50	0.46
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.98	0.46
1:A:3526:PRO:C	1:A:3528:ALA:H	2.23	0.46
1:A:586:GLN:HB2	1:A:613:HIS:CD2	2.51	0.45
1:A:1086:TYR:C	1:A:1088:GLU:H	2.22	0.45
1:A:189:MET:SD	1:A:189:MET:N	2.90	0.45
1:A:4020:MET:HE2	1:A:4020:MET:HA	1.99	0.45
1:A:2365:ASN:ND2	1:A:2396:LEU:HD13	2.27	0.45
1:A:3779:SER:OG	1:A:3780:ALA:N	2.50	0.45
1:A:225:LYS:HZ3	1:A:253:LEU:HD13	1.81	0.45
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	1.99	0.45
1:A:2164:TRP:C	1:A:2167:PRO:HD2	2.42	0.45
1:A:180:LEU:HA	1:A:230:LEU:HD21	1.97	0.45
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.17	0.45
1:A:487:LEU:HD12	1:A:490:ILE:HD11	1.99	0.45
1:A:3186:ARG:HD3	1:A:3238:MET:CE	2.44	0.45
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.98	0.45
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.98	0.45
1:A:2252:PRO:C	1:A:2254:ARG:H	2.24	0.45
1:A:2576:MET:HB3	1:A:2787:HIS:CD2	2.52	0.45
1:A:3369:ASP:OD1	1:A:3369:ASP:N	2.49	0.45
1:A:2408:MET:HE3	1:A:2411:LEU:HD22	1.98	0.45
1:A:3478:GLU:CD	1:A:3478:GLU:N	2.75	0.45
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.99	0.45
1:A:1221:ILE:HD12	1:A:1221:ILE:H	1.82	0.45
1:A:2372:PRO:O	1:A:2374:LEU:N	2.50	0.45
1:A:3444:ALA:CB	1:A:3482:LEU:CD2	2.93	0.45
1:A:1572:LEU:HB3	1:A:1614:GLN:HE21	1.81	0.45
1:A:2539:LEU:HD13	1:A:2562:LEU:HD11	1.97	0.45
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.98	0.45
1:A:3410:ILE:HD11	1:A:3456:LEU:HB3	1.98	0.45
1:A:3922:ASP:O	1:A:3923:ARG:NE	2.49	0.45
1:A:3484:THR:HG23	1:A:3513:ALA:HA	1.97	0.45
1:A:1124:ILE:HG23	1:A:1182:GLU:HG2	1.99	0.44
1:A:3793:VAL:HG13	1:A:3803:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:SER:O	1:A:1482:GLU:HG3	2.17	0.44
1:A:3636:PHE:CE2	1:A:3670:MET:HG2	2.52	0.44
1:A:1019:ASP:HA	1:A:1026:ARG:HH11	1.83	0.44
1:A:1458:LEU:HD13	1:A:1467:ILE:HD11	2.00	0.44
1:A:3467:ARG:O	1:A:3471:ILE:HG12	2.17	0.44
1:A:3925:LEU:HD23	1:A:3925:LEU:HA	1.75	0.44
1:A:4127:TRP:CD1	1:A:4128:MET:H	2.35	0.44
1:A:154:SER:HA	1:A:157:TYR:HD2	1.82	0.44
1:A:275:PHE:CZ	1:A:293:LEU:HD21	2.53	0.44
1:A:1538:LEU:HD12	1:A:1553:PHE:CE1	2.52	0.44
1:A:1864:ASP:N	1:A:1864:ASP:OD1	2.50	0.44
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.99	0.44
1:A:2411:LEU:C	1:A:2413:PHE:H	2.24	0.44
1:A:2945:SER:HB2	1:A:2946:GLU:OE1	2.17	0.44
1:A:849:GLU:OE2	1:A:852:ARG:NH1	2.50	0.44
1:A:1640:GLU:OE1	1:A:1640:GLU:N	2.50	0.44
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.52	0.44
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.98	0.44
1:A:2575:PRO:HA	1:A:2786:LYS:H	1.83	0.44
1:A:2849:SER:O	1:A:2849:SER:OG	2.36	0.44
1:A:3575:LEU:HD23	1:A:3575:LEU:HA	1.81	0.44
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.50	0.44
1:A:1300:SER:O	1:A:1300:SER:OG	2.32	0.44
1:A:3088:LEU:HD23	1:A:3088:LEU:HA	1.74	0.44
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.99	0.44
1:A:131:LEU:HD12	1:A:132:ILE:N	2.33	0.44
1:A:151:GLU:HB3	1:A:153:PHE:CE1	2.53	0.44
1:A:396:PHE:HB3	1:A:441:MET:HE1	1.99	0.44
1:A:2863:CYS:SG	1:A:2895:GLU:HG3	2.57	0.44
1:A:3878:VAL:HG21	1:A:4128:MET:HB3	1.98	0.44
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.99	0.44
1:A:1636:ASP:N	1:A:1636:ASP:OD1	2.50	0.44
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.98	0.44
1:A:2097:LEU:HD23	1:A:2097:LEU:HA	1.81	0.44
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.83	0.44
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.44
1:A:225:LYS:HZ3	1:A:253:LEU:HD22	1.82	0.43
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.51	0.43
1:A:2443:MET:C	1:A:2445:LYS:H	2.25	0.43
1:A:2887:PRO:HB2	1:A:3895:GLU:HG3	2.00	0.43
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3981:TYR:HB2	1:A:4108:MET:HE1	2.00	0.43
1:A:4107:LEU:HD23	1:A:4107:LEU:HA	1.79	0.43
1:A:1427:SER:O	1:A:1431:LEU:HD23	2.18	0.43
1:A:1820:VAL:HG12	1:A:1824:LEU:HD23	2.00	0.43
1:A:493:LYS:O	1:A:625:ASN:ND2	2.51	0.43
1:A:671:SER:O	1:A:675:ARG:HG3	2.18	0.43
1:A:3603:LYS:HB3	1:A:3606:ILE:HG22	1.98	0.43
1:A:59:PHE:O	1:A:63:PHE:N	2.52	0.43
1:A:1770:GLN:N	1:A:1770:GLN:OE1	2.51	0.43
1:A:2522:ARG:HG2	1:A:2561:PHE:CE1	2.52	0.43
1:A:3383:GLN:O	1:A:3387:GLU:HG3	2.17	0.43
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	2.00	0.43
1:A:1802:TYR:O	1:A:1806:ARG:HG2	2.19	0.43
1:A:3523:ASP:OD1	1:A:3561:LYS:NZ	2.31	0.43
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.52	0.43
1:A:1627:LYS:HD2	1:A:1627:LYS:HA	1.83	0.43
1:A:3604:LYS:HA	1:A:3607:GLU:HG2	2.00	0.43
1:A:3655:LYS:C	1:A:3657:SER:H	2.26	0.43
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.51	0.43
1:A:79:ARG:O	1:A:82:ARG:HB2	2.19	0.43
1:A:1365:ASN:OD1	1:A:1366:THR:N	2.51	0.43
1:A:1586:SER:O	1:A:1586:SER:OG	2.34	0.43
1:A:2554:PHE:C	1:A:2556:SER:H	2.27	0.43
1:A:174:VAL:O	1:A:177:LEU:HG	2.18	0.43
1:A:253:LEU:HD12	1:A:254:LYS:N	2.34	0.43
1:A:346:TYR:HD1	1:A:366:TYR:HH	1.66	0.43
1:A:2466:SER:C	1:A:2468:THR:H	2.27	0.43
1:A:221:ALA:O	1:A:225:LYS:HE3	2.18	0.43
1:A:853:ILE:HA	1:A:3111:MET:HE1	2.00	0.43
1:A:2220:MET:HB3	1:A:2255:LEU:HD22	2.01	0.43
1:A:3858:MET:HE3	1:A:3858:MET:HB3	1.88	0.43
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.80	0.43
1:A:563:LEU:O	1:A:567:GLU:HG2	2.19	0.43
1:A:1192:TYR:OH	1:A:1275:THR:OG1	2.35	0.43
1:A:1391:VAL:HG13	1:A:1392:MET:SD	2.59	0.43
1:A:1622:ILE:HG21	1:A:1652:ILE:HD11	2.00	0.43
1:A:3176:MET:HE2	1:A:3246:ALA:HB2	2.00	0.43
1:A:287:LEU:HG	1:A:326:MET:SD	2.59	0.42
1:A:958:MET:HE3	1:A:958:MET:HB2	1.86	0.42
1:A:1220:LEU:O	1:A:1223:THR:OG1	2.27	0.42
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1557:GLU:CA	1:A:1592:MET:HE1	2.49	0.42
1:A:1935:GLU:OE2	1:A:1938:ARG:NE	2.34	0.42
1:A:2415:LEU:HD12	1:A:2420:PHE:CG	2.53	0.42
1:A:2531:LEU:HD12	1:A:2531:LEU:HA	1.88	0.42
1:A:3227:ILE:O	1:A:3228:SER:HB3	2.19	0.42
1:A:466:LEU:HB3	1:A:560:LEU:HD22	2.01	0.42
1:A:1218:SER:O	1:A:1222:ASN:ND2	2.52	0.42
1:A:2347:LYS:C	1:A:2351:GLN:HE22	2.27	0.42
1:A:3542:PHE:HZ	1:A:3555:VAL:HG11	1.84	0.42
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.93	0.42
1:A:192:ASN:OD1	1:A:192:ASN:N	2.52	0.42
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.72	0.42
1:A:1308:ALA:C	1:A:1310:GLU:H	2.28	0.42
1:A:1714:LEU:HD23	1:A:1714:LEU:HA	1.86	0.42
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.52	0.42
1:A:3843:LEU:HD21	1:A:3858:MET:HE2	2.00	0.42
1:A:240:GLU:HB3	1:A:242:PRO:HD2	2.01	0.42
1:A:469:ALA:HB2	1:A:479:ILE:HD11	2.02	0.42
1:A:737:PRO:HD2	1:A:740:ILE:HD12	2.01	0.42
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	2.01	0.42
1:A:1496:GLU:OE1	1:A:1496:GLU:N	2.42	0.42
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	2.01	0.42
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	2.01	0.42
1:A:1395:LEU:O	1:A:1398:VAL:HG22	2.20	0.42
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.20	0.42
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	2.01	0.42
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.34	0.42
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.19	0.42
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	2.01	0.42
1:A:128:LEU:HD13	1:A:131:LEU:HD21	2.02	0.42
1:A:355:ASN:OD1	1:A:356:ASN:N	2.52	0.42
1:A:623:PHE:CE2	1:A:665:GLY:HA3	2.54	0.42
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.34	0.42
1:A:236:LYS:HD3	1:A:246:ARG:HH12	1.84	0.42
1:A:523:THR:HG23	1:A:525:LYS:H	1.85	0.42
1:A:1242:LEU:HA	1:A:1310:GLU:HB2	2.01	0.42
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.20	0.42
1:A:3229:SER:OG	1:A:3232:ARG:NH1	2.43	0.42
1:A:3318:LYS:O	1:A:3322:ALA:HB3	2.19	0.42
1:A:3829:LEU:HD23	1:A:3829:LEU:HA	1.92	0.42
1:A:3846:MET:HE2	1:A:3846:MET:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3875:GLU:O	1:A:3878:VAL:HG12	2.19	0.42
1:A:3917:ILE:HD13	1:A:4051:LEU:HD21	2.00	0.42
1:A:109:ASN:OD1	1:A:110:THR:N	2.53	0.42
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.28	0.42
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	2.01	0.42
1:A:3138:ILE:O	1:A:3142:ILE:HG12	2.20	0.42
1:A:3271:ASP:HB2	1:A:3315:TYR:CE2	2.55	0.42
1:A:42:CYS:HA	1:A:88:PHE:CE1	2.55	0.42
1:A:195:ASN:OD1	1:A:196:LEU:N	2.52	0.42
1:A:935:HIS:NE2	1:A:939:MET:HE2	2.34	0.42
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.01	0.42
1:A:4015:ASN:O	1:A:4018:GLN:HG3	2.20	0.42
1:A:12:LEU:HA	1:A:15:LEU:HB3	2.00	0.42
1:A:60:SER:OG	1:A:61:ARG:N	2.53	0.42
1:A:251:PHE:HA	1:A:254:LYS:NZ	2.35	0.41
1:A:1431:LEU:HD11	1:A:1447:ARG:NH2	2.35	0.41
1:A:31:GLY:HA2	1:A:34:LEU:HB2	2.03	0.41
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.90	0.41
1:A:1424:THR:HG23	1:A:1427:SER:H	1.85	0.41
1:A:1871:MET:O	1:A:1875:LYS:HG3	2.20	0.41
1:A:2802:PRO:HG2	1:A:2803:ILE:HD12	2.02	0.41
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.19	0.41
1:A:3477:GLU:N	1:A:3477:GLU:CD	2.78	0.41
1:A:29:LEU:HD13	1:A:32:HIS:HB3	2.02	0.41
1:A:442:GLN:HG3	1:A:461:ILE:HD11	2.02	0.41
1:A:888:ARG:HB3	1:A:3889:ARG:HH21	1.85	0.41
1:A:995:PHE:HB3	1:A:1005:ASP:OD1	2.19	0.41
1:A:1374:GLN:HE22	1:A:1381:SER:CB	2.33	0.41
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.20	0.41
1:A:2771:LEU:HD12	1:A:2775:TYR:HE2	1.85	0.41
1:A:220:LEU:O	1:A:224:LEU:HG	2.21	0.41
1:A:3537:SER:HA	1:A:3540:TYR:CE2	2.55	0.41
1:A:202:GLY:HA2	1:A:205:LYS:HE2	2.02	0.41
1:A:1538:LEU:HD12	1:A:1553:PHE:HE1	1.86	0.41
1:A:1575:LEU:HD11	1:A:1617:LYS:HG3	2.03	0.41
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.35	0.41
1:A:3791:TYR:HB3	1:A:3806:LEU:HD21	2.02	0.41
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	2.02	0.41
1:A:36:ARG:NE	1:A:36:ARG:HA	2.36	0.41
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	2.02	0.41
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3816:LEU:HD21	1:A:3883:LEU:HD13	2.01	0.41
1:A:275:PHE:HZ	1:A:293:LEU:HD21	1.84	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1261:LEU:CD1	1:A:1340:ARG:HG3	2.51	0.41
1:A:1795:VAL:HG21	1:A:1838:GLU:HG3	2.03	0.41
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.56	0.41
1:A:2492:ASP:C	1:A:2494:ASP:H	2.28	0.41
1:A:3687:MET:HB3	1:A:3722:PHE:CD1	2.56	0.41
1:A:68:PHE:O	1:A:71:LYS:HB2	2.21	0.41
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.85	0.41
1:A:1219:PHE:O	1:A:1223:THR:HG23	2.21	0.41
1:A:35:ILE:HG21	1:A:80:GLU:HB3	2.02	0.41
1:A:296:VAL:HG23	1:A:297:LEU:HD12	2.03	0.41
1:A:1240:THR:HG23	1:A:1296:PHE:CG	2.56	0.41
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.20	0.41
1:A:1836:LEU:HD21	1:A:1883:ARG:HH21	1.85	0.41
1:A:2339:GLU:HG2	1:A:2340:SER:N	2.36	0.41
1:A:2392:VAL:O	1:A:2396:LEU:HD23	2.21	0.41
1:A:3012:GLU:HB2	1:A:3047:SER:HB2	2.02	0.41
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	2.03	0.41
1:A:3227:ILE:HG22	1:A:3228:SER:N	2.36	0.41
1:A:3692:VAL:HG13	1:A:3692:VAL:O	2.21	0.41
1:A:3843:LEU:HD23	1:A:3843:LEU:HA	1.87	0.41
1:A:397:LEU:HD22	1:A:437:HIS:HB3	2.03	0.41
1:A:1348:LEU:HD23	1:A:1348:LEU:HA	1.84	0.41
1:A:2231:PHE:O	1:A:2235:LEU:HD23	2.21	0.41
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.56	0.41
1:A:2392:VAL:HG12	1:A:2396:LEU:HD23	2.03	0.41
1:A:3959:MET:HE3	1:A:3959:MET:H	1.86	0.41
1:A:2578:GLU:H	1:A:2578:GLU:CD	2.29	0.40
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.20	0.40
1:A:3483:MET:O	1:A:3483:MET:HG3	2.16	0.40
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.86	0.40
1:A:1445:ARG:HG3	1:A:1510:LEU:HD13	2.03	0.40
1:A:1589:ASN:C	1:A:1591:LYS:H	2.29	0.40
1:A:2305:ASN:O	1:A:2308:SER:OG	2.34	0.40
1:A:3091:LEU:HD23	1:A:3091:LEU:HA	1.88	0.40
1:A:3505:LEU:HD23	1:A:3505:LEU:H	1.86	0.40
1:A:1754:GLN:HE22	1:A:1788:ARG:HD2	1.86	0.40
1:A:2133:LEU:HD23	1:A:2164:TRP:CZ3	2.56	0.40
1:A:2776:ARG:NE	1:A:2782:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LYS:HB2	1:A:474:VAL:HB	2.04	0.40
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.21	0.40
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.40
1:A:2122:LEU:HD12	1:A:2122:LEU:HA	1.93	0.40
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.21	0.40
1:A:249:PHE:O	1:A:252:VAL:HG12	2.21	0.40
1:A:1504:ASP:C	1:A:1506:SER:H	2.30	0.40
1:A:1790:SER:O	1:A:1794:GLN:HG3	2.21	0.40
1:A:2165:LEU:HA	1:A:2165:LEU:HD12	1.81	0.40
1:A:2823:PHE:CD2	1:A:2824:LYS:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3640/4156 (88%)	3332 (92%)	304 (8%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	1968	SER
1	A	1813	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3234/3671 (88%)	3230 (100%)	4 (0%)	88 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2105	HIS
1	A	3477	GLU
1	A	3478	GLU
1	A	3483	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	A	325	ASN
1	A	334	HIS
1	A	484	HIS
1	A	869	ASN
1	A	1083	ASN
1	A	1222	ASN
1	A	1426	GLN
1	A	1457	GLN
1	A	1552	HIS
1	A	1574	ASN
1	A	1771	GLN
1	A	2091	HIS
1	A	2283	ASN
1	A	2305	ASN
1	A	2351	GLN
1	A	2365	ASN
1	A	2422	GLN
1	A	2514	ASN
1	A	2553	HIS
1	A	2784	GLN
1	A	2954	GLN
1	A	3093	GLN
1	A	3122	HIS
1	A	3139	GLN
1	A	3154	GLN

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Mol	Chain	Res	Type
1	A	3422	GLN
1	A	3470	GLN
1	A	3515	GLN
1	A	3787	GLN
1	A	3903	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	95.34
1	A	5016:UNK	C	6001:UNK	N	49.10

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11185. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.